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Abstract

Selectivity Enhancement of an Acetone-Monitoring SPR Sensor: Theoretical Evaluation †

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Abstract: A numerical investigation of a sensor for acetone monitoring using surface plasmon resonance (SPR) is proposed. We evaluate the effects of polyaniline (PANI), graphene, or chitosan acting as a chemisorption binding layer for the selective sensing of acetone. Our findings suggest that these materials present suitable responses when applied as an overlayer to the sensor. Their thicknesses, however, should be maintained close to a monolayer level to preserve performance.

Keywords: acetone sensor; surface plasmon resonance; adsorption; volatile organic compound

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1. Introduction

Acetone is a volatile organic compound that has been the subject of attention in human exhaled breath applications, working as a biomarker for metabolic changes in individuals affected by some diseases, like diabetes [1]. However, the heterogeneity of compounds present in the exhaled breath causes acetone detection to become a challenge. Research in the area aims to find materials to interface this specific analyte with sensor structures. The pursued objective is to detect acetone molecules while avoiding other compounds. The purpose of this paper is to provide an analysis of the materials that have been tested for their chemisorption properties concerning acetone but were not thoroughly applied in conjunction with SPR instrumentation.

2. Materials and Methods

For the numerical analysis, we used a Kretschmann–Raether setup. The calculations were conducted based on the Fresnel equations. Firstly, we simulated and chose parameters for the optimal substrate and metal layers considering the refractive index of acetone. Gold (Au) or silver (Ag) were evaluated for the metal layer. The analyte (acetone) was simulated as a bulk of 150 nm. We simulated our target molecule as if it were contained in an aqueous matrix of breath condensate. Our initial sensor used polycarbonate with a fixed thickness of 3 mm for the optical substrate. Finally, the wavelengths were set to 800 nm for gold and 662 nm for silver. The SPR curve parameters achieved by this initial setup are written in the two first lines of Table 1. The objective was to compare bare-gold- and bare-silver-based SPR sensors to the configurations with the addition of the acetone-binding materials.

Table 1. Results for sensor layer simulations.

Layers	Thickness	FHWM	MRR	RA
Bare gold	51 nm	0.865	<0.001	63.5°
Bare silver	57 nm	0.406	<0.001	63.7°
Gold/chitosan	1 nm (chitosan)	0.865	<0.001	63.58°
Gold/graphene	1 nm (graphene)	0.915	0.08	63.98°
Gold/PANI	1 nm (PANI)	0.881	0.17	63.05°
Silver/chitosan	1 nm (chitosan)	0.406	<0.001	63.82°
Silver/graphene	1 nm (graphene)	0.437	0.27	64.30°
Silver/PANI	1 nm (PANI)	0.436	0.22	63.49°

3. Discussion

The results are shown in Table 1. Silver achieved the best performance among the metals. Although silver is susceptible to oxidation [2], the added affinity layers may serve as protection against such an effect. Based on the best result, we plotted the SPR signal of the silver-based sensor as a function of the affinity layer thickness, as shown in Figure 1. The most significant repercussion due to the use of PANI was an increase in the minimum reflectance at resonance (MRR) for both metals. This impact was proportional to the thickness of the PANI layer. For silver and gold, the average increase in the MRR was 0.22 and 0.17 per nm of PANI, respectively. The changes in the full width at half maximum (FWHM) and the resonance angle (RA) were slight. Graphene, in turn, caused an increase in the MRR but in conjunction with a displacement of the resonance angle to the right. Finally, using chitosan did not cause modifications to the MRR or FWHM but only a displacement of the resonance angle to the right. In this sense, chitosan is the best-performing acetone affinity layer. For all affinity layers, their thicknesses should be maintained as close to their monolayer levels as possible. As their thicknesses increased, degradations in the SPR curve also increased. The use of chitosan, PANI, and graphene is promising, according to our results. Derived from these preliminary results, the experimental setup of an exhaled breath condensed detector is under development.

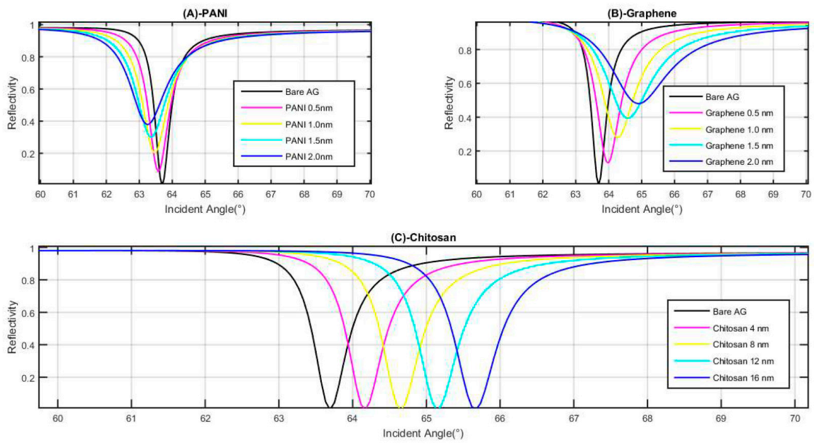

Figure 1. SPR curves for silver-based sensor as a function of affinity layer thickness.

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